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**PREDICTING DIFFUSION OF ATMOSPHERIC
CONTAMINANTS BY CONSIDERATION OF
TURBULENT CHARACTERISTICS OF WSMR**

By
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ATMOSPHERIC SCIENCES LABORATORY
WHITE SANDS MISSILE RANGE, NEW MEXICO

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CLASSIFICATION

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ABSTRACT

The relationships between the turbulent intensities about the mean flow in the lowest layers of the atmosphere at White Sands Missile Range, New Mexico, and climatological data are discussed in terms of predicting the diffusion of contaminants into the atmosphere. If the turbulent fluctuations observed in the lower portion of the boundary layer are considered representative, then correlations with climatological summaries may be used as a rudimentary estimator for estimating the diffusion power of the atmosphere. A simple empirical diffusion model for general use is also given.

CONTENTS

	Page
ABSTRACT -----	iii
INTRODUCTION -----	1
PURPOSE OF DIFFUSION STUDY -----	2
THE SITE -----	2
TURBULENT CHARACTERISTICS OF WSMR -----	2
TERRAIN EFFECTS ON THE MEAN WIND -----	15
AN EMPIRICAL DIFFUSION PREDICTION MODEL -----	15
DISCUSSION AND SUMMARY -----	23
REFERENCES -----	24

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INTRODUCTION

Diffusion of aerosols and particulate matter into the atmosphere from an instantaneous or continuous point source can be adequately predicted over short distances if restrictions are placed on the prediction model. Since problems of diffusion are of an individualistic nature, i.e., the conditions for diffusion vary from locale to locale, prediction schemes are normally determined empirically for a specific location and are based upon the theoretical models of Hay and Pasquill [1959] or Sutton [1932, 1934, 1947].

The development of a prediction scheme normally involves detailed studies of the area in question with respect to the meteorological and climatological characteristics and the use of tracer materials and detection systems to determine dispersion patterns. The actual field testing is normally easy to accomplish; however, the extraction of intelligence from the resulting data in terms of the meteorological situation are sometimes meaningless and obscure. The major causes of a poor data fit to theoretical considerations usually stem from the fact that the prediction models are based upon stationary conditions and homogeneous underlying terrain. Since most locations where there is a diffusion problem are less than ideal from a meteorological standpoint, the empirical solutions for atmospheric dispersion of gases or matter are necessarily based upon gross statistics and regression techniques and fail to account for the heterogeneous effects that lead to prediction errors that can over- or underestimate by a factor of two to four.

The scatter about a regression curve can be considered a measure of nonuniform effects upon the dispersion of contaminants into the atmosphere. The processes determining the heterogeneity of flow across a surface are not completely understood; consequently, it is difficult to compensate for this in terms of diffusion theory and its application. Thus, timely and realistic predictions of dispersion corridors and concentrations of contaminants at any point downstream of the source must necessarily be in the three-sigma range to allow for the effects of nonhomogeneous conditions.

A diffusion study for any locale, then, must include a micrometeorological study that considers all factors of the mean flow in steady and nonsteady state conditions and over a wide stability range. The vertical fluxes of heat, momentum, and matter into the atmosphere, and of course all the other turbulent parameters must be determined for the particular surface over which the diffusion will occur. Surface

discontinuities that cause horizontal gradients and nonequilibrium profiles and fluxes great distances downstream must be compensated for in the analysis of test data.

PURPOSE OF DIFFUSION STUDY

The Atmospheric Sciences Laboratory, White Sands Missile Range (WSMR), New Mexico, is currently engaged in a study of the meteorological factors that affect the diffusion of toxic liquid propellants into the atmosphere. The purpose of the study is to provide the National Aeronautics and Space Administration White Sands Test Facility (WSTF) with timely and representative information concerning possible hazard corridors and concentration of toxic vapors in the vicinity of the Apollo site.

The purpose of this paper is to present some preliminary data concerning the characteristics of the planetary boundary layer that may be applied to diffusion into the atmosphere. Also included is an empirical diffusion model that may be used with some success over a rough, nonhomogeneous terrain.

THE SITE

White Sands Missile Range is located in South-Central New Mexico, almost wholly in the Tularosa Basin. The western boundaries of the range extend across the San Andres Range of the southern Rockies into the eastern portion of the Rio Grande Valley and the Jornada Del Muerto. The Apollo site is located on the western slopes of the San Andres and is mainly on the talus of the mountain range which is characterized by numerous arroyos, rocky soil, and sparse vegetation. The locale is heterogeneous from the micrometeorological standpoint. Man-made obstructions such as buildings and other modifications to the terrain contribute to the overall heterogeneity.

TURBULENT CHARACTERISTICS OF WSMR

The diffusive power of the atmosphere is directly related to the turbulent characteristics of the planetary boundary layer, and particularly to the vertical temperature gradient, the mean wind speed and the direction. The logical starting point, then, of any diffusion study is to review the turbulent characteristics of the atmosphere for the locale in question; keeping in mind of course, the differences that may exist owing to possible separation of the data collection site and the area of interest.

The investigation of the turbulent characteristics in the vicinity of WSMR has been quite productive in that large data samples have been collected and thoroughly analysed. A goodly portion of the data are applicable to the Apollo side of the mountains, even though they were collected in the Tularosa basin portion of WSMR.

It has been shown by Monin-Obukhov [1954], Panofsky [1961, 1963] Ellison [1957] and others that atmospheric turbulence obeys the laws of dynamic similarity of flows. In the surface boundary layer and to lesser extent in the planetary boundary layer proper, the wind and temperature profiles can be shown to be given by, respectively,

$$\frac{z}{L} = S Ri K_H/K_M \quad (1)$$

and

$$\frac{z}{L} = R Ri (K_H/K_M)^2 \quad (2)$$

where z/L is the Monin-Obukhov scaling ratio, Ri is the gradient Richardson number, S is a dimensionless wind shear, R is a dimensionless lapse rate and K_H/K_M is the ratio of the exchange coefficients for heat and momentum. Batchelor [1953] has shown that the Richardson number is the basic parameter of similarity for the boundary layer, and it has been demonstrated by Hansen [1966], and Swanson and Cramer [1965] that the turbulent characteristics of the boundary layer are directly related to this basic stability parameter. The Richardson number is usually expressed as

$$Ri = \frac{g}{\bar{\theta}} \frac{\partial \bar{\theta} / \partial z}{(\partial \bar{V} / \partial z)^2} \quad (3)$$

where g is the acceleration of gravity, $\bar{\theta}$ is potential temperature, \bar{V} is the mean horizontal wind speed and z is height. From the similarity theory it may be shown that the Richardson number is also a function of height and its vertical distribution governed by

$$(Ri)' = \frac{\sum Ri(z)}{\sum z(j)} \quad (4)$$

$$j = 1, 2, 3, 4, \dots$$

where $(Ri)'$ denotes the height derivative of Ri . An investigation of the distribution of Ri with time as well as height by Hansen and Lang [1966] reveals that eq. (4) adequately describes the height distribution of Ri to the top of the surface boundary layer which, depending upon stability, is some 10 to 40 meters above the surface. This is shown in Figures 1 and 2 for both homogeneous and nonhomogeneous flow conditions. Figures 1 and 2 reveal that critical values of Ri exist, especially in the unstable regime. It has been found by Dyer [1965] and Hansen [1967] that critical Ri is in the range $-0.70 > Ri > -1.2$. In the stable regime, critical Ri is thought to lie between $Ri = 0.20$ and $Ri = 0.40$. Outside these limits are regimes of local nonstationarity known as the "undulant" regime for very stable conditions and the "windless convection" regime for the extremely unstable case.

It was also found that temporally the distribution of Ri with height was as depicted in Figure 3. It is seen that the Richardson number varies with the energy balance of the boundary layer, which is best shown in Figure 4. From Figures 3 and 4 it is seen that the atmosphere is almost wholly thermally stratified at all times and that neutral conditions exist only for very short periods near sunrise and sunset. It is interesting to note that the Richardson number at 3 and 6 meters is almost perfectly correlated with the incoming short wave and net radiation curves, indicating that the stability of the atmosphere at these heights reflects steady-state conditions much better than some other reference height, say 1.5 meters.

If the basic similarity parameter is taken to be the Richardson number, and if it is taken to be an independent variable in the boundary layer, eqs. (1) and (2) may be integrated to find the wind and temperature profiles. Substituting in and integrating eq. (1) yields

$$V = \frac{u_*}{k} \left[\ln \frac{z}{z_0} - \psi(z/L) \right] \quad (5)$$

which is known as the log-linear wind profile, where u_* is a stress term, k is Karman's constant, z_0 is the roughness length and $\psi(z/L)$ is a universal function. A similar expression may be written for the temperature profile, although not in such a universal form. The turbulent characteristics of the boundary layer may then be expressed as deviations about the mean profile as functions of Ri .

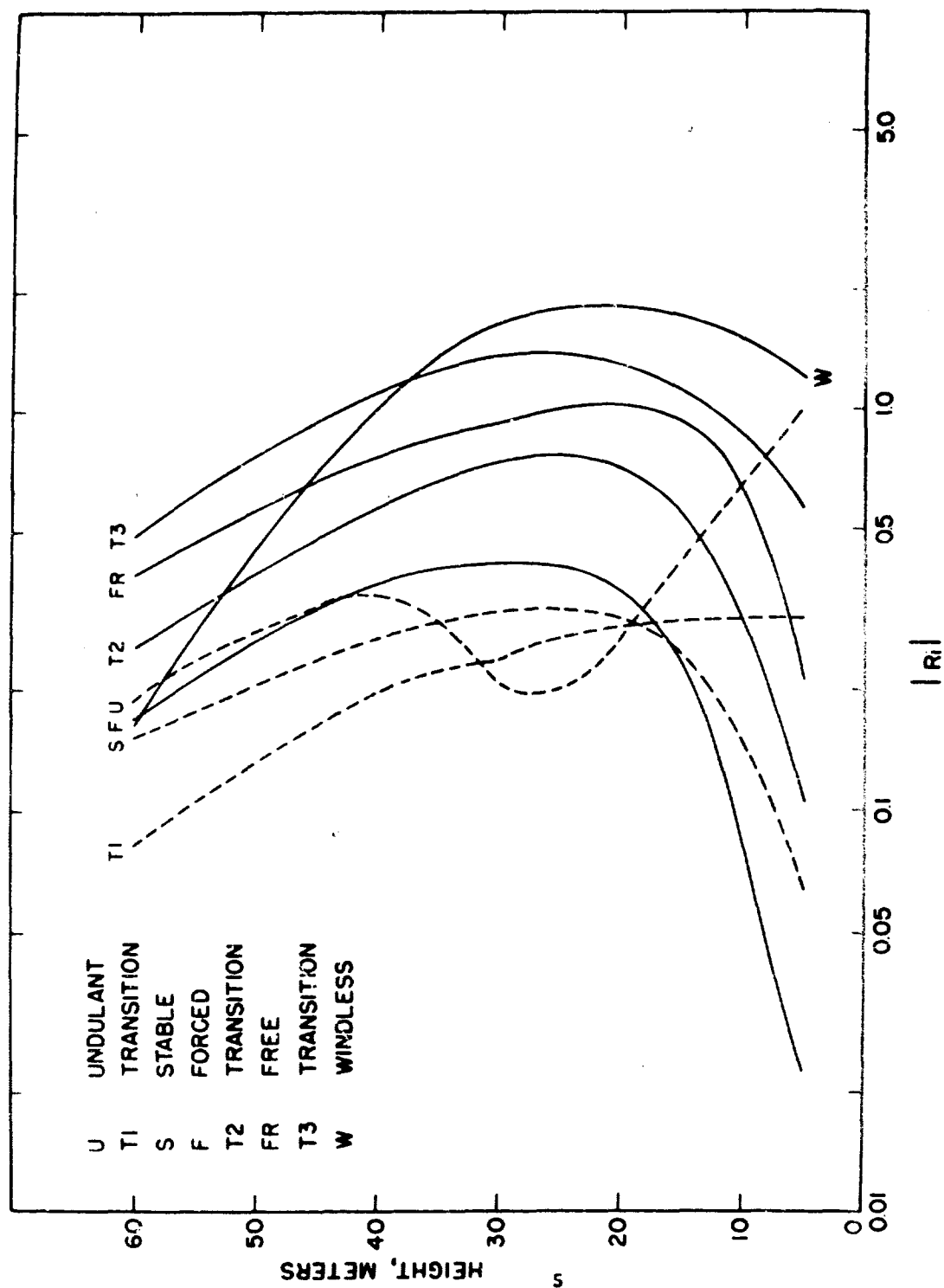


FIG 1 ABSOLUTE VALUE OF THE RICHARDSON NUMBER VS HEIGHT FOR EIGHT STABILITY CONDITIONS FOR HOMOGENEOUS FLOW.

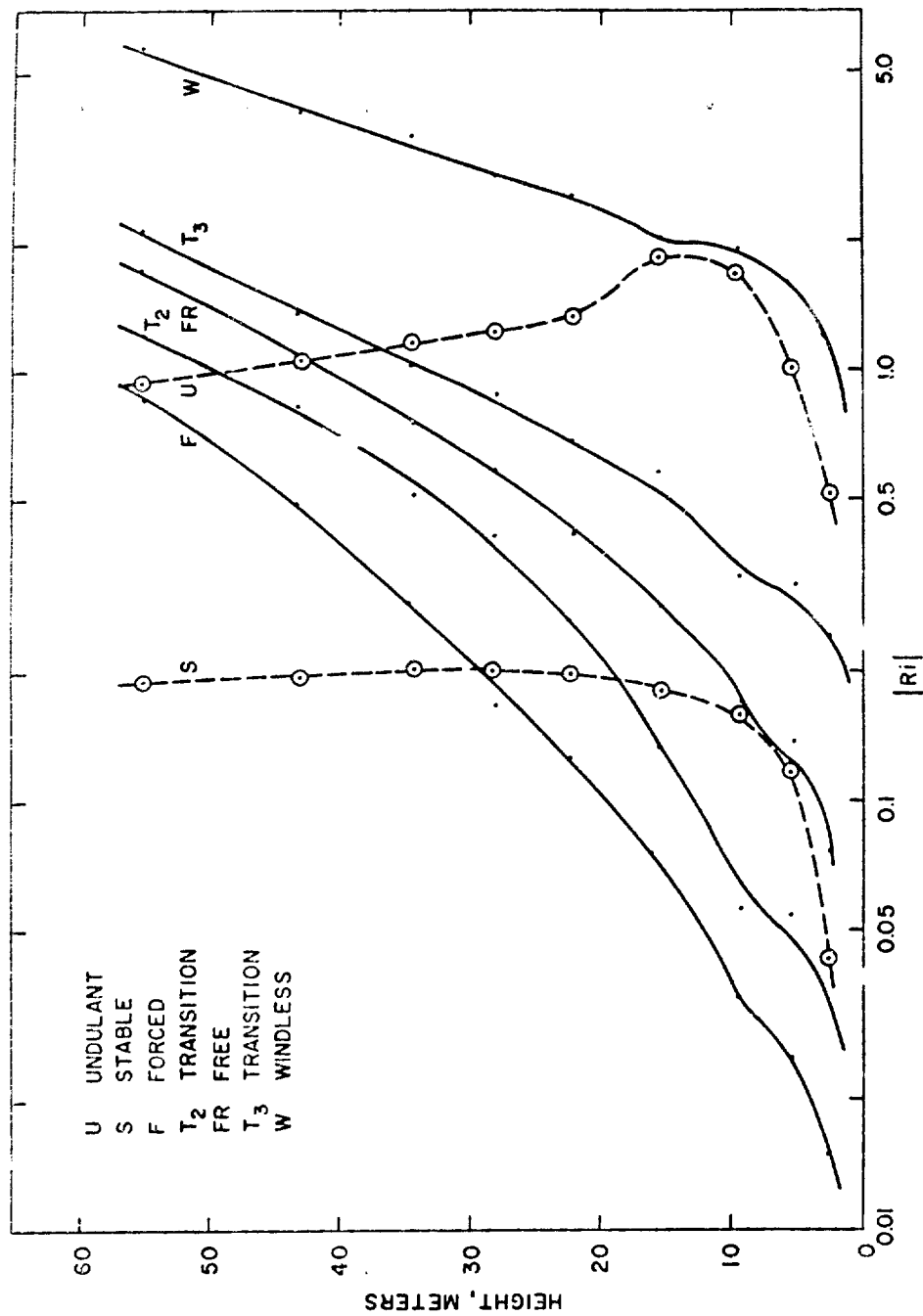


FIGURE 2 ABSOLUTE VALUE OF THE RICHARDSON NUMBER VERSUS HEIGHT FOR SEVEN STABILITY CONDITIONS FOR NONHOMOGENEOUS FLOW.

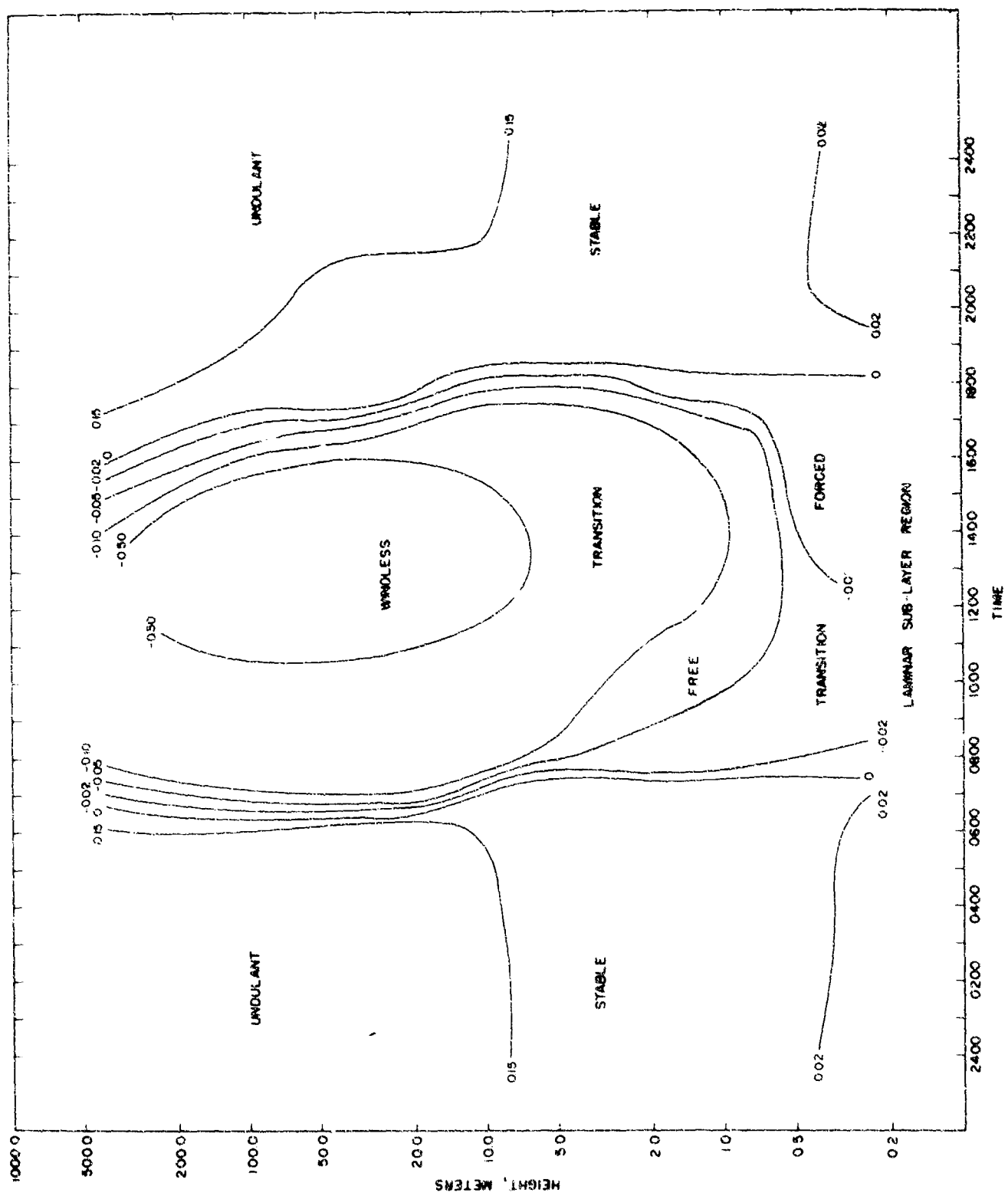


FIG 3 THE RICHARDSON NUMBER AS A FUNCTION OF HEIGHT AND TIME

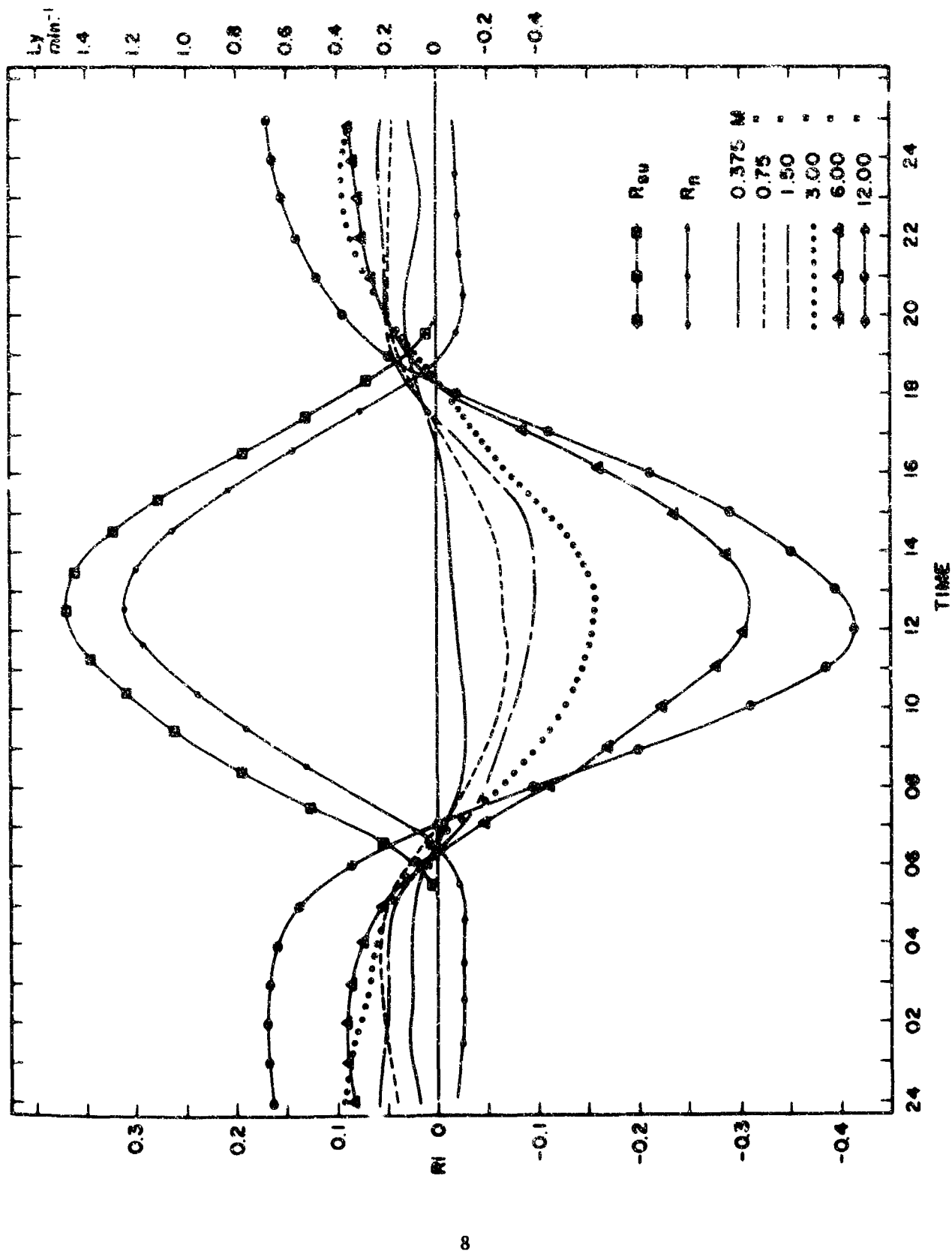


FIG. 4 THE RICHARDSON NR. AT SELECTED HEIGHTS VERSUS NET AND INCOMING SHORT-WAVE RADIATION.

Swanson and Cramer [1965], Hansen [1966] and Hansen and Lang [1967] have shown that the turbulent wind and temperature fluctuations about the means are directly related to the stability regime. It was found that the orthogonal components of the horizontal wind were functions of stability and to a lesser extent functions of surface roughness. The turbulent intensity was also found to be height dependent in the form

$$G_x, G_y = Cz^p \quad (6)$$

where G_x and G_y are defined as

$$G_x = \sigma u' / \bar{V} \quad (7)$$

$$G_y = \sigma v' / \bar{V} \approx \sigma A_R \quad (8)$$

where $\sigma u'$ and $\sigma v'$ are the standard deviations of the longitudinal and lateral eddy velocities and σA_R is the standard deviation about the mean wind direction in radians. The constant C is a function of surface roughness while the exponent p is related to the exponent of the conjugate power law wind profile and is a function of Ri .

Hansen and Lang's [1967] results are shown in Figures 5 through 8. It will be noted that an inflection occurs in the σA versus z regression of Figure 8 for the stable case. This is attributed to a surface roughness discontinuity upstream of the research tower as reported by Hansen and Hansen [1965]. The inflection in the curve is the result of excessive surface stress downstream of the discontinuity and the lack of vertical transport of momentum in stable flow conditions through the internal momentum boundary.

Turbulent temperature fluctuations over a nonhomogeneous surface are shown in Figure 9 as a function of the Richardson number. It is seen that in the region below the internal momentum boundary the quantity $\sigma T / \partial \theta / \partial z$ does not exhibit the predicted characteristics as indicated by Tsvang [1960] and Lumley and Panofsky [1964]. Above the interface height of 8 to 10 meters, the scaling temperature $T^*(T^* \propto \sigma T / \partial \theta / \partial z)$ has the predictable characteristic of being nearly unity in unstable flow and independent of height in stable conditions. The dashed portions of this curve indicate local nonstationarity

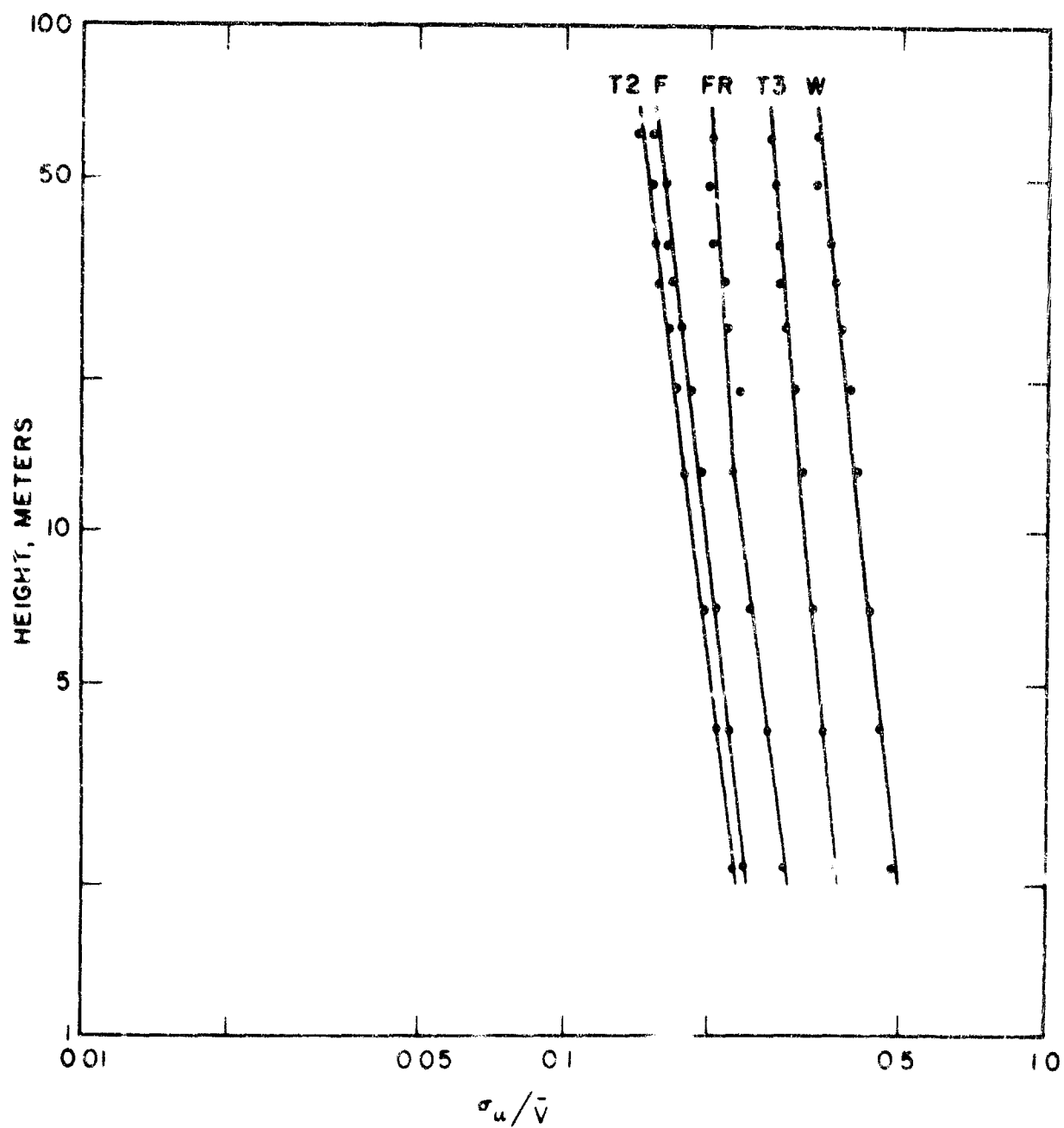


FIGURE 5 HEIGHT DEPENDENCE OF THE LONGITUDINAL INTENSITY OF TURBULENCE DURING UNSTABLE STRATIFICATION.

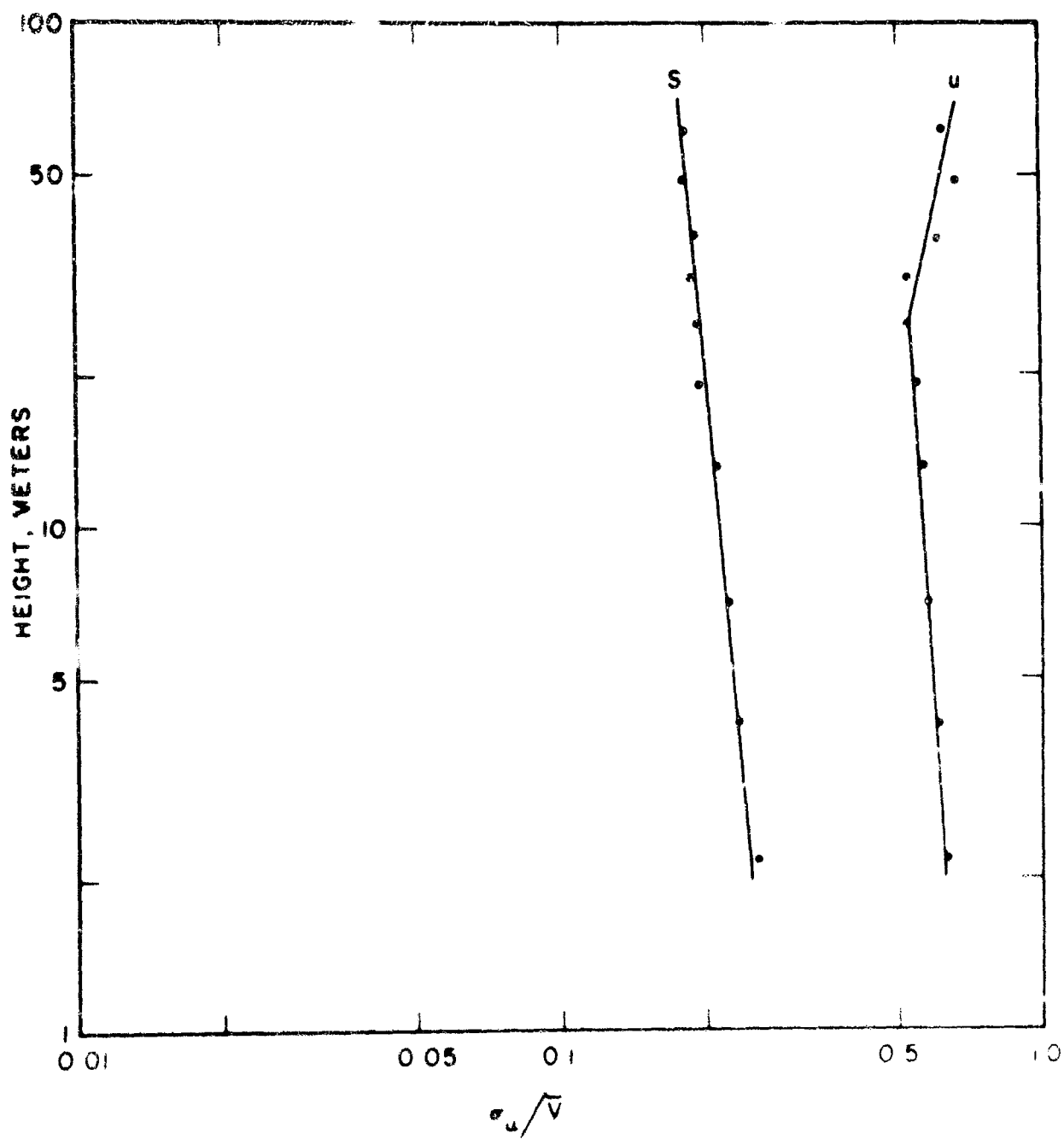


FIGURE 6 HEIGHT DEPENDENCE OF THE LONGITUDINAL INTENSITY OF TURBULENCE DURING STABLE STRATIFICATION

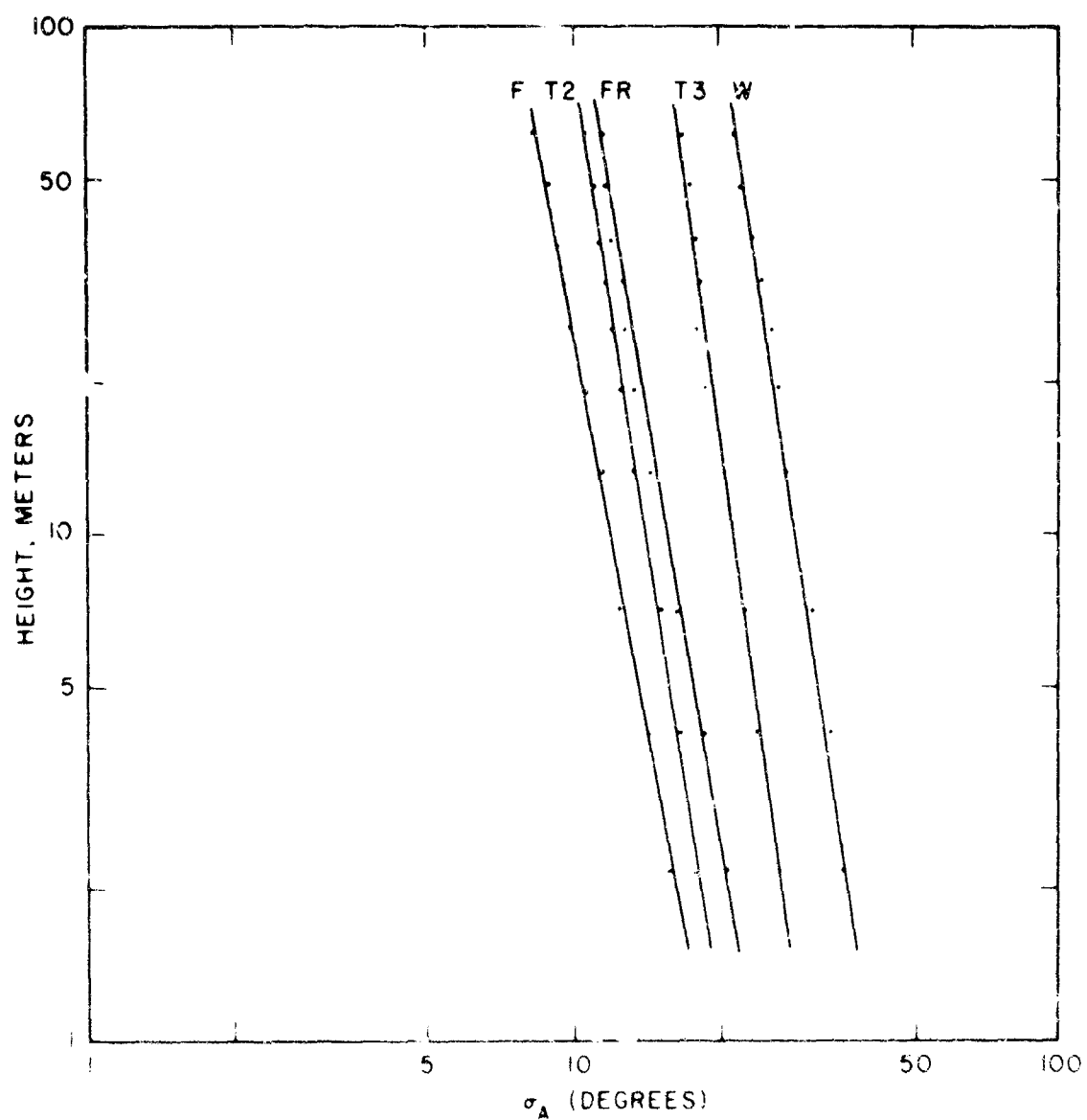


FIGURE 7 HEIGHT DEPENDENCE OF THE LATERAL INTENSITY OF TURBULENCE DURING UNSTABLE STRATIFICATION

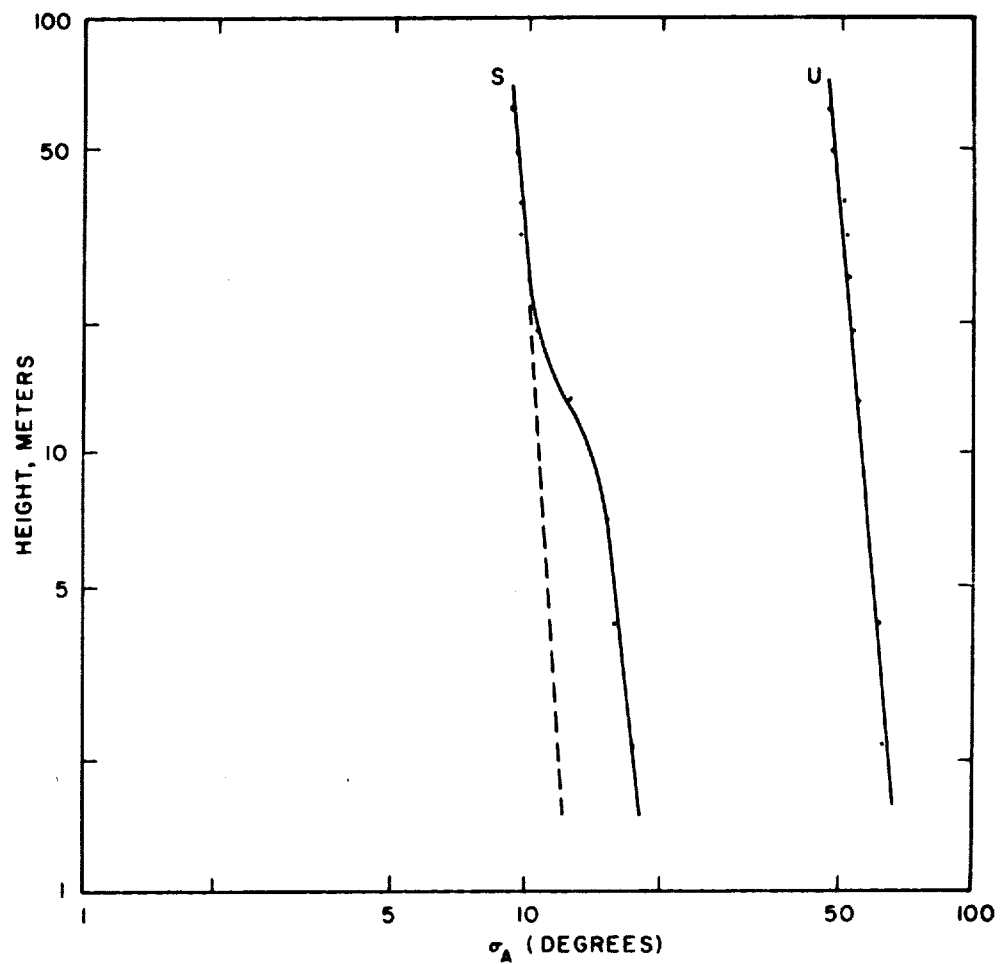


FIGURE 8 HEIGHT DEPENDENCE OF THE LATERAL INTENSITY OF TURBULENCE DURING STABLE STRATIFICATION

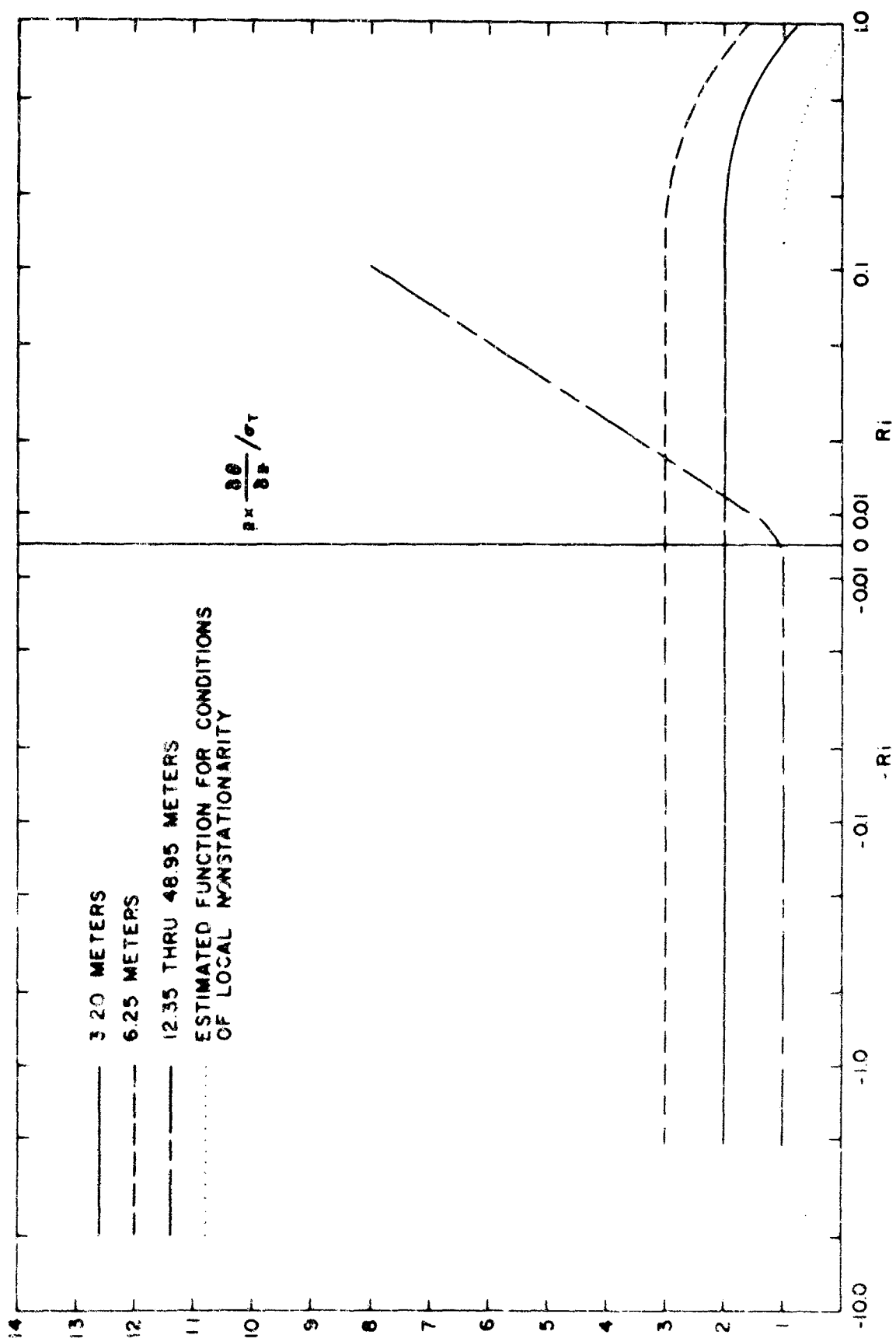


FIGURE 9 T^*/σ_T AS A FUNCTION OF THE RICHARDSON NUMBER

effects upon the experimental data. On the stable side, it appears that undulance has the same effects as the nonequilibrium flow beneath the boundary.

TERRAIN EFFECTS ON THE MEAN WIND

The terrain of WSMR and particularly the proximity of a mountain range to the experimental site has a profound effect upon the annual wind regime at WSMR. Hansen and Lang [1966b, 1966c] found that the annual wind regime could be expressed in terms of three seasonal regimes. These consisted of a winter regime, a two-part spring regime and a combined summer-fall regime. The winter and spring seasons are characterized by generally strong westerly flow with the summer-fall regime being generally southeasterly. All seasons reflect a significant percentage of drainage winds from the mountain slopes during the nocturnal hours. The percent frequency of occurrence of wind direction for all seasons is shown in Figures 10 through 13.

Other terrain effects such as the roughness length have been investigated. Hansen [1967] has found that the roughness length of the terrain about the research tower varies with wind direction and with the season. The seasonal change in roughness is shown in Figure 14. It will be noted that the curve approximates the growing season in that the largest values of z_0 are found in July and August when the vegetive canopy is most dense.

AN EMPIRICAL DIFFUSION PREDICTION MODEL

Experimental evidence shows that three meteorological parameters should be considered in characterizing the rate of small scale atmospheric diffusion:

(1) The mean wind speed \bar{V} as an indicator of the downstream travel of the plume emitted from a continuous source.

(2) The standard deviation of wind direction σ_A as an indicator of the lateral rate of mixing.

(3) The temperature gradient ΔT as an indicator of the vertical rate of mixing.

Other quantities of interest are the peak or maximum concentration C_p at some distance x downstream of the source and the related source

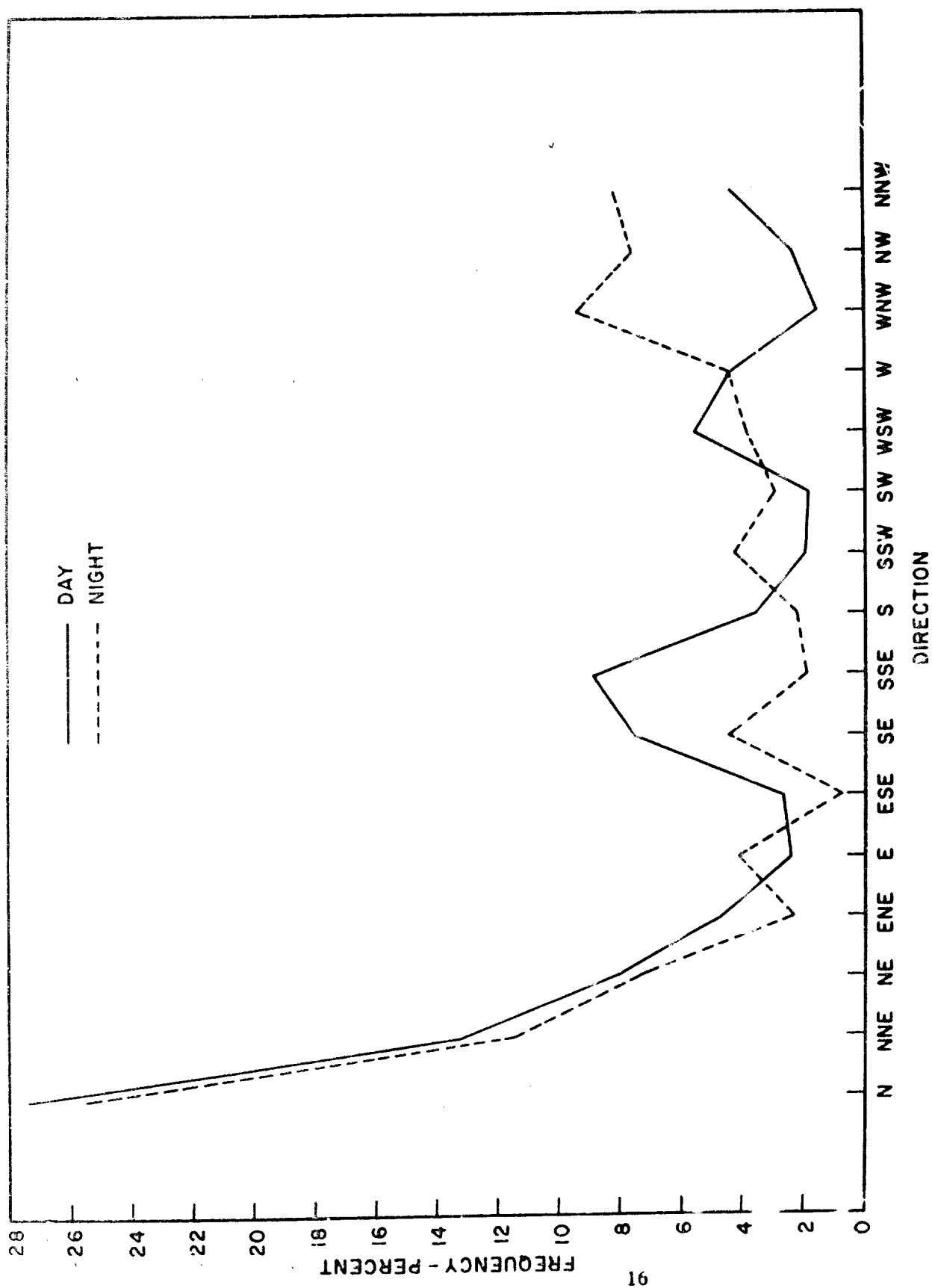


FIGURE 10 PERCENT FREQUENCY OF OCCURRENCE OF WIND DIRECTION, WINTER

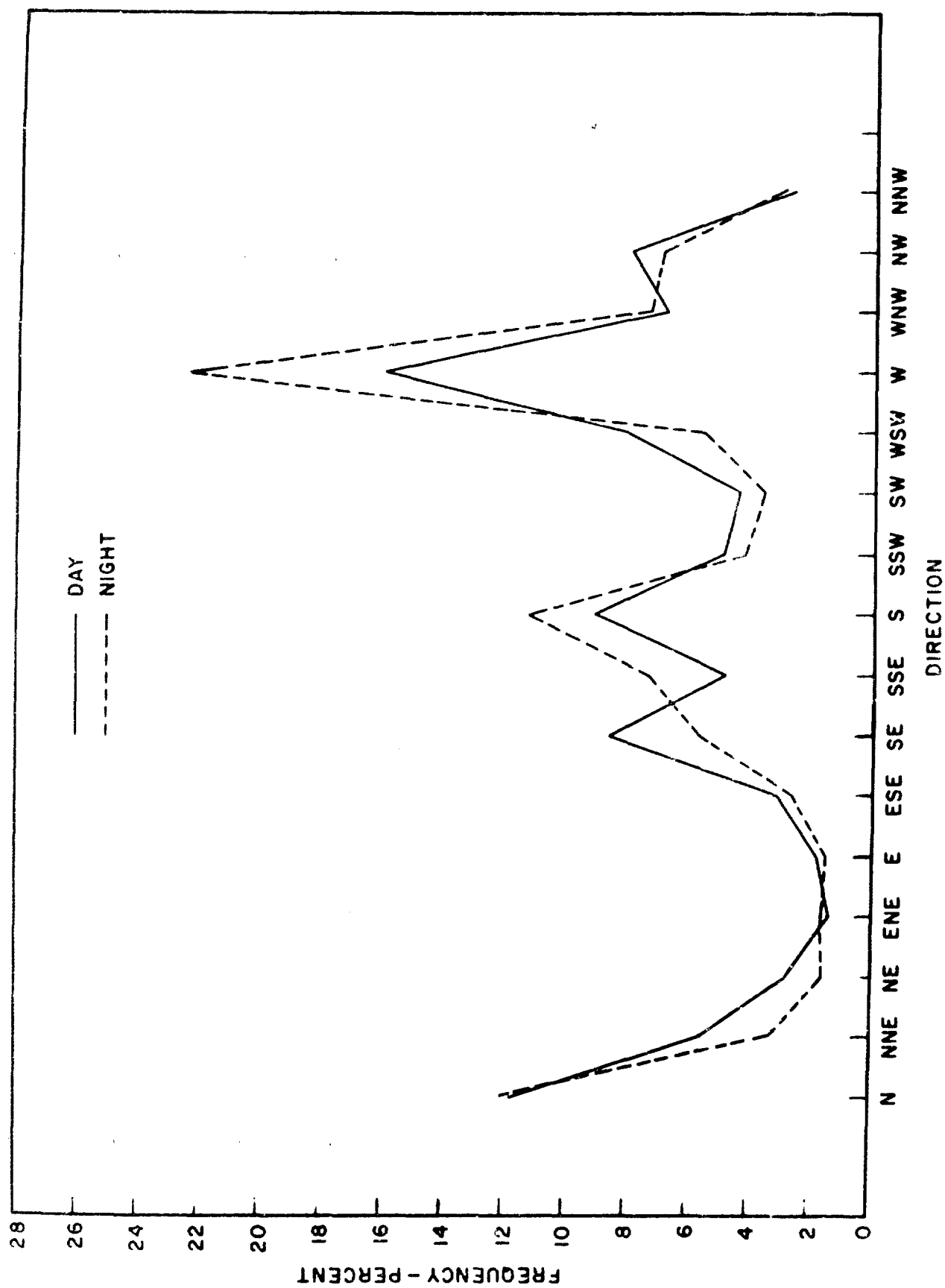


FIGURE II PERCENT FREQUENCY OF OCCURRENCE OF WIND DIRECTION, SPRING (PART I)

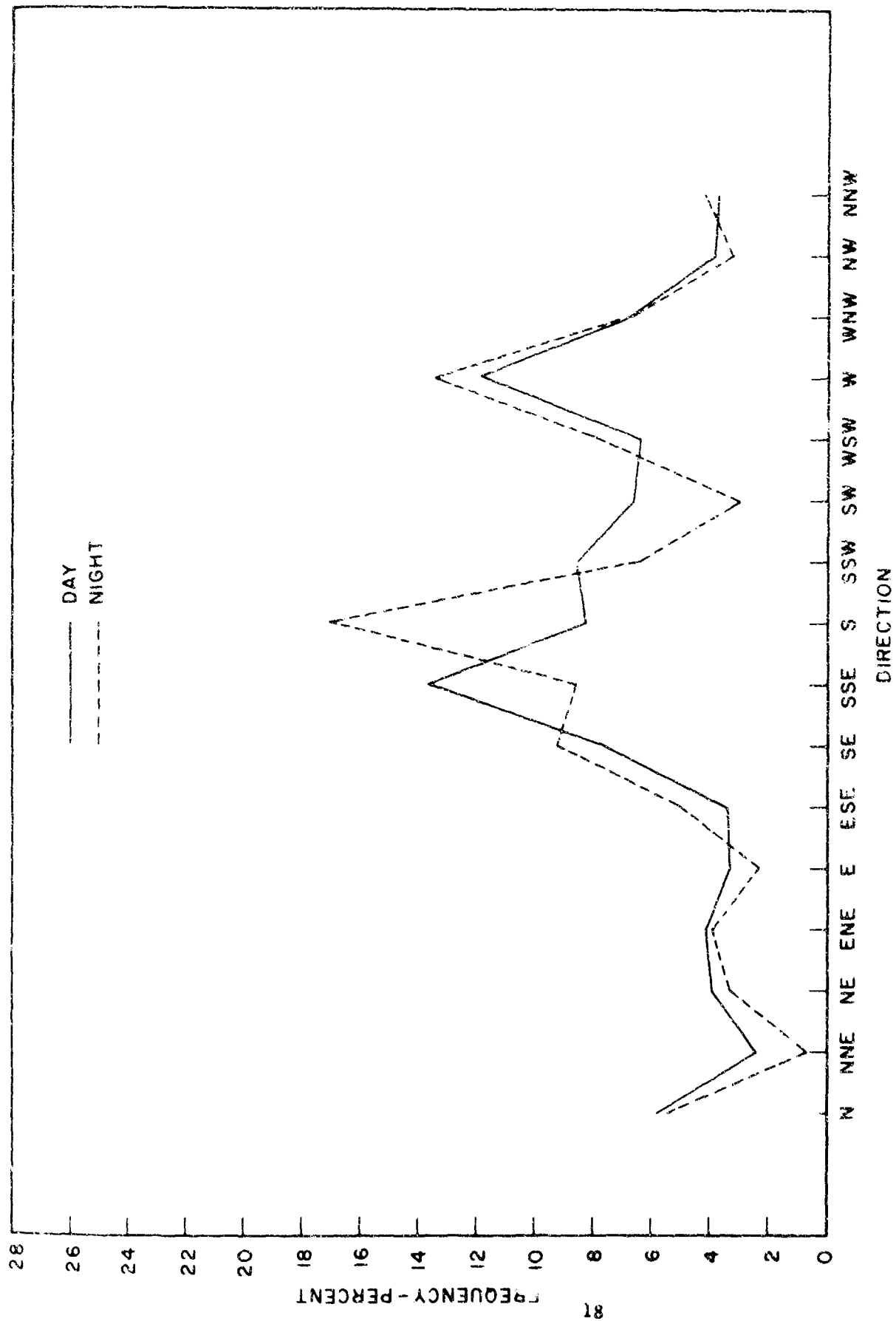


FIGURE 12 PERCENT FREQUENCY OF OCCURRENCE OF WIND DIRECTION, SPRING (PART 2)

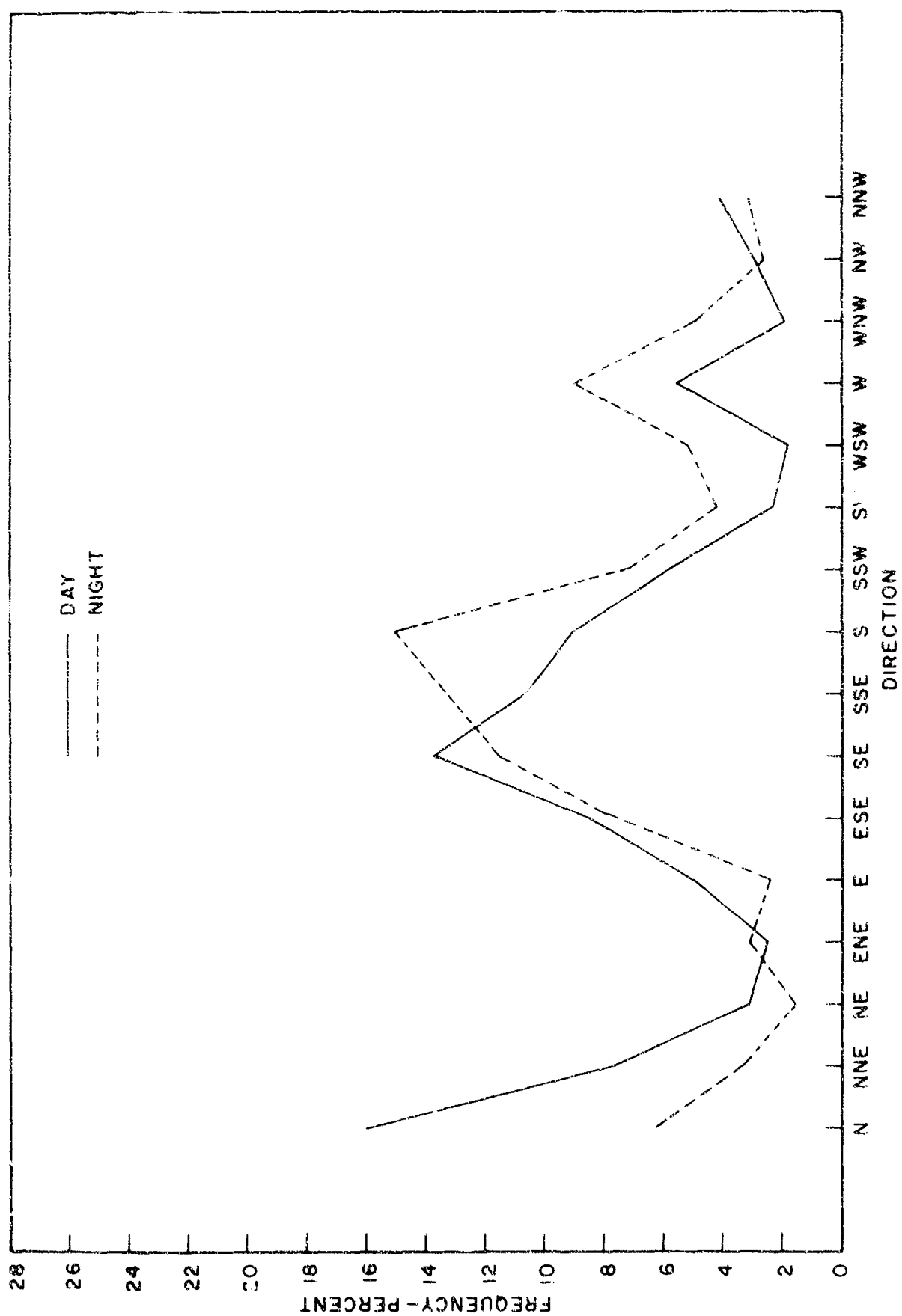


FIGURE 13 PERCENT FREQUENCY OF OCCURRENCE OF WIND DIRECTION, SUMMER - FALL

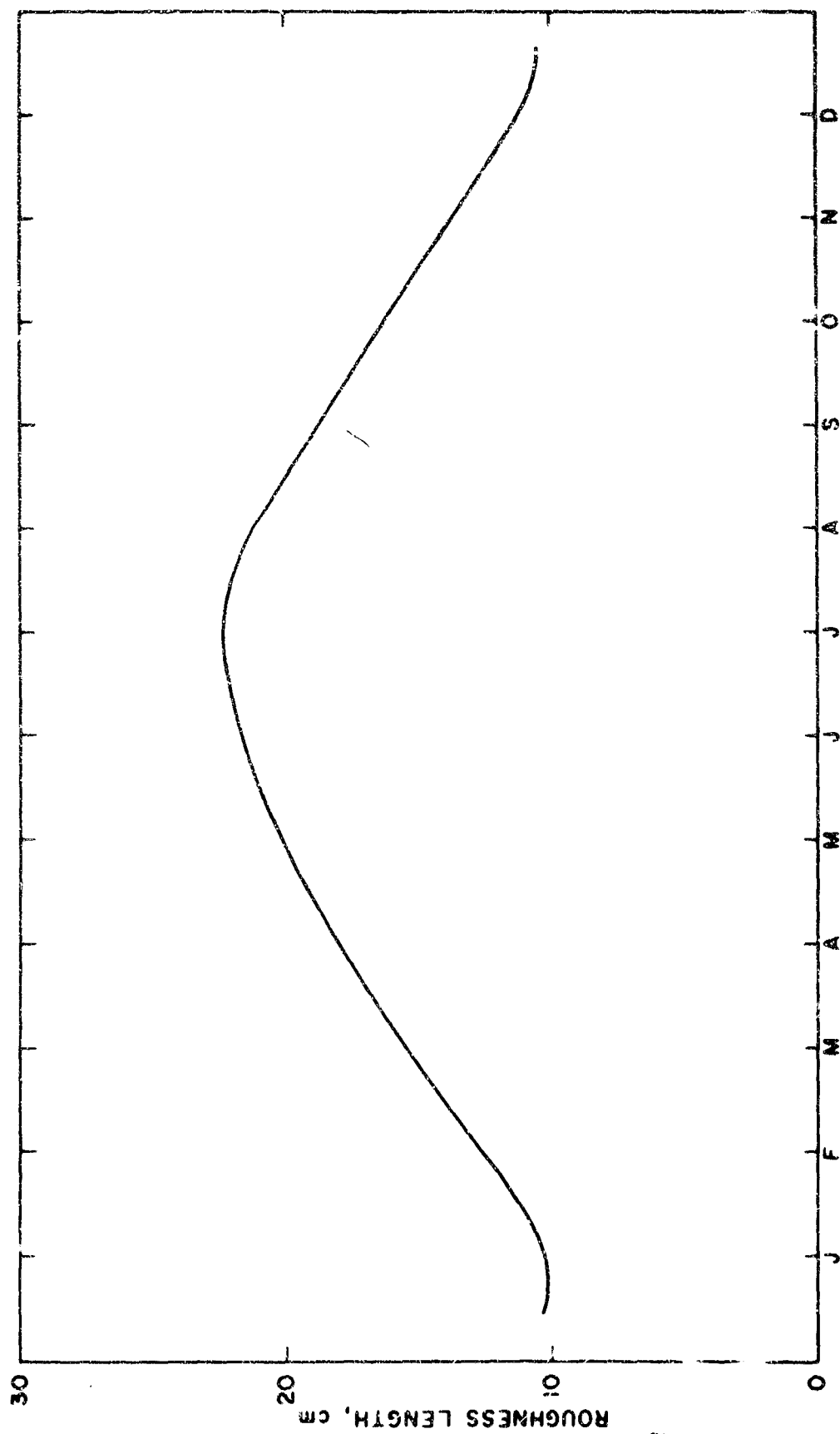


FIGURE 14 THE AVERAGE ROUGHNESS LENGTH BY MONTH FOR WHITE SANDS MISSILE RANGE, NEW MEXICO.

strength Q . In the development of a regression equation for predicting diffusion, a normalized peak concentration C_p/Q at distance x is generally the goal.

The regression equation usually takes the form

$$C_p/Q = Kx^a \bar{V}^b \sigma A^c (\Delta T+t)^d \quad (9)$$

where K , a , b , c , d are parameters of fit and t is a constant added to ΔT to avoid raising a negative number to a power.

Application of linear multiple regression techniques requires taking the logarithm of eq (9) and applying standard least-squares analysis to the following:

$$\log C_p/Q = \log K + a \log x + b \log \bar{V} + c \log \sigma A + d \log (\Delta T+t) \quad (10)$$

since the normalized peak concentration could be linear with respect to the meteorological variables but not linear in distances.

A general purpose form of equation (9) for use in nonhomogeneous terrain has been developed by Miller and Miller [1963] in the form

$$C_p/Q = 0.000175 x^{-1.95} (\Delta T+10)^{4.95} \quad (11)$$

where C_p is the peak concentration in gms m^{-3} at a height of about 1.5 meters above the surface at a downwind travel distance, x , in meters, Q is the source strength in gm sec^{-1} and ΔT is the temperature difference in deg. F between 16.5 and 1.8 meters above the ground. Eq. (11) was developed from experimental data simulating ground-level continuous point sources.

It will be noted that the mean wind speed \bar{V} and the standard deviation of wind direction are not included in eq. (11). It was found by Haugen and Taylor [1963] and Miller and Miller [1963] that while \bar{V} is correlated with C_p/Q , its contribution to the predictability after the temperature differential is included was not significant. The σA term was dropped owing to the fact that no satisfactory

method of obtaining σA from an analogue recorder was available. Estimates for σA will be introduced below.

For direct application, eq (11) must be converted to units which may be used conveniently. The conversion is relatively simple for contaminants emitted as a ground-level continuous point source. In the case of a gaseous contaminant, C_p/Q should be known in terms of parts per million of the contaminant per pound per minute released into the atmosphere, a value that is dependent upon the diffusive power of the atmosphere and the physical characteristics of the contaminant. Under standard conditions, 1 ppm $lb^{-1} min$ equals the gram molecular weight of the gas times $5.89 \times 10^{-6} sec m^{-3}$. To obtain parts per million per pound per minute, C_p/Q in $sec m^{-3}$, is multiplied by 1.70×10^5 and divided by the gram molecular weight.

In terms of travel distance for normalized peak concentrations eq (11) may be restated as

$$x(\text{in feet}) = 2.62(C_p/Q)^{-0.513} [\Delta T + 10]^{2.53} \quad (12)$$

and

$$x(\text{in feet}) = 2.20 (C_p/Q)^{-0.513} [\Delta T + 10]^{2.53} \quad (13)$$

Eqs. (12) and (13) are valid for two well-known propellants, nitrogen tetroxide and unsymmetrical dimethylhydrazine. For other fuels or oxidizers, the constants of eqs. (12) and (13) must be modified according to the scheme outlined above.

Travel time of the contaminant to a particular location can be determined from the mean wind speed. The width of the hazard corridor can be estimated from a wind direction trace by

$$W = C R \quad (14)$$

where W is the width of the corridor, R is the range of the wind direction, and C is an empirical constant determined for a locale and a particular recorder speed. Eq. (14) yields equivalent results obtained by Haugen and Taylor [1963] who showed that the width of the hazard corridor could be estimated from $W = 8 \sigma A$ with 95% confidence that this value would not be exceeded.

DISCUSSION AND SUMMARY

If the turbulent characteristics of the boundary layer as observed at WSMR can be considered typical of an area that includes the WSTF (Apollo) locale, some insight into the diffusion of a contaminant into the atmosphere is provided. If the WSMR turbulence intensities are typical, then climatological type data at WSTF may be used to investigate the diffusive power of the atmosphere, alleviating any need for elaborate multilevel tower systems which are a necessity at WSMR.

The only exception to this approach would be the drainage wind pattern during the nocturnal hours. It is clear that the drainage pattern at WSTF would not be the same as it is at WSMR. This is because WSMR and WSTF are on opposite slopes of the mountain range. It appears likely that the nocturnal drainage on the western slopes of the San Andres would be almost a mirror image of the eastern slope drainage pattern with few exceptions.

The use of the Miller and Miller [1963] diffusion equation for predicting concentrations and hazard corridors for WSTF is perhaps not completely justified but is a useful tool for estimating the dispersion of contaminants in the atmosphere. The development of a more precise empirical model for WSTF would entail a very complex and costly experiment.

This analysis indicates that the turbulent characteristics of the atmosphere as observed at White Sands are representative of larger areas. Under these conditions then, the diffusive power of the atmosphere at the Apollo site may be estimated from rudimentary climatological data used in conjunction with the WSMR data.

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13. ABSTRACT <p>The relationships between the turbulent intensities about the mean flow in the lowest layers of the atmosphere at White Sands Missile Range, New Mexico, and climatological data are discussed in terms of predicting the diffusion of contaminants into the atmosphere. If the turbulent fluctuations observed in the lower portion of the boundary layer are considered representative, then correlations with climatological summaries may be used as a rudimentary estimator for estimating the diffusion power of the atmosphere. A simple empirical diffusion model for general use is also given.</p>		

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14	KEY WORDS	LINK A		LINK B		LINK C	
		ROLE	WT	ROLE	WT	ROLE	WT
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